

AMENDMENTS TO THE SPECIFICATION

Please replace paragraph [0014] with the replacement paragraph below.

[0014] The accompanying drawings, which are incorporated into and constitute a part of the specification, illustrate specific embodiments of the invention and, together with the general description of the invention given above, and the detailed description of the specific embodiments, serve to explain the principles of the invention.

FIG. 1 is a flow chart illustrating an embodiment of the present invention.

FIG. 2 shows a strip chart used to plot output from the standard structure comparison analysis of protein structures. FIG. 2 is Figure 1A in the journal article LGA: a method for finding 3D similarities in protein structures by Adam Zemla, in the journal, Nucleic Acids Research, 2003, Vol. 31, No. 13, pp. 3370-3374.

FIG. 3 shows the strip chart representing the results from the LGA analysis (the regions of the structure deviation are clearly detected). FIG. 3 is Figure 1B in the journal article LGA: a method for finding 3D similarities in protein structures by Adam Zemla, in the journal, Nucleic Acids Research, 2003, Vol. 31, No. 13, pp. 3370-3374.

FIG. 4 illustrates 3D plot (backbone representation) of the structure superposition of two structures. Plot corresponds to the fourth strip bar from the Fig. 2.

FIG. 5 illustrates 3D plot (backbone representation) of the structure superposition of two structures. Plot corresponds to the fourth strip bar from the Fig. 3. representing the results from the LGA analysis.

FIG. 6 is a bar representation of the results from sequence independent LGA superpositions. FIG. 6 is Figure 2A in the journal article LGA: a method for finding 3D similarities in protein structures by Adam Zemla, in the journal, Nucleic Acids Research, 2003, Vol. 31, No. 13, pp. 3370-3374.

FIG. 7 shows regions of structural similarity in 3D plot (backbone representation) between the reference structure.

Please replace paragraph [0036] with the replacement paragraph below.

[0036] For given two protein structures the present invention provides a method of finding regions of 3D similarities in protein structures between a first molecule and a second molecule. The method comprises a number of following steps. Comparing the first molecule and the second molecule using Longest Continuous Segments (LCS) analysis. Comparing the first molecule and the second molecule using Global Distance Test (GDT) analysis. Evaluating the calculated alignment between the first molecule and the second molecule using Local Global Alignment Scoring function (LGA_S). For many different alignments repeating the steps above to find the complete set of local and global regions of 3D similarities between given two protein structures. The Local Global Alignment Scoring function (LGA_S) is described in greater detail in the following portions of the DETAILED DESCRIPTION OF THE INVENTION, particularly in paragraph [0036]. The journal article LGA: a method for finding 3D similarities in protein structures by Adam Zemla, in the journal, Nucleic Acids Research, 2003, Vol. 31, No. 13, pp. 3370-3374 includes a section under the heading "Description of the LGA scoring function" which provides additional information about using Local Global Alignment Scoring function (LGA_S). The journal article LGA: a method for finding 3D similarities in protein structures by

Adam Zemla, in the journal, Nucleic Acids Research, 2003, Vol. 31, No. 13, pp. 3370-3374 is incorporated herein in its entirety by this reference.

9